tallized at 4 °C for 1 day. As a result, a white powder with a humidity of 10 % and a specific rotation $[\alpha]_D = -36.5°$ was obtained. The purity of inulin was monitored by chromatography on paper in a solvent system of butanol-acetic acid-water 4 : 1 : 2.

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HYDROGEN BONDS BETWEEN PYRIDINE AND HALOFORMS – NEW INSIGHTS

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Pyridine has not only been recognized as an important solvent in the organic synthesis, but also an essential building block of most drugs [1, 2]. Understand of the pyridine involved hydrogen bond, its strength under various conditions, its impact on the vibrations of the participating molecules is critical in the organic synthesis, molecular scaffold study in drug design, as well as in the study of the properties of pyridine containing biological ligands [3–5]. In nearly all the hydrogen bonding relationship that pyridine has ever involved, it is mainly considered as the electron lone pair donor, in other word, hydrogen bonding acceptor [6, 7].

With the formation of the hydrogen bond, the electron density on the pyridine ring will naturally experience redistribution in different degrees depending on the strength of the hydrogen bond. This electron density redistribution generally leads to a frequency shift of the ring related vibrations [8–10]. Among 27 vibrational normal modes of pyridine, ring breathing vibration ν_1 and triangle vibration ν_{12} have been extensively investigated with respect of their response to the hydrogen bonding [11–14].

In the present work hydrogen bond between pyridine (Py) and haloforms (CHX_3, X = F, Cl, Br, I) was studied using a combination of solution phase FTIR and quantum mechanical ab initio calculations. All FTIR measurements were performed at room temperature (298±2 K) and cyclohexane used to record the background spectra. The infrared absorption spectra of solutions with concentration of 1 M and mixtures with different volumetric ratios were recorded on a ThermoScientific Nicolet iS5 FT-IR Spectrometer using KBr windows with a 1 cm^{-1} resolution over the range of 400–4000 cm^{-1}. Calculations were performed in Gaussian09 with DFT ωB97X-D/6-311++G** (H, C, N) / DGDZTP (X) functional. While the calculation indicates other than the hydrogen bond formed between pyridinyl nitrogen ([Py–]N) and the H atom on haloform ($[CX_3–]$H), a ring structure is established based on both the [Py–]N involved hydrogen bond and the interaction between the alpha H on pyridine ([Py–]H) and the halogen atom on haloform ($[CHX_2–]$X). The formation of the ring makes the entire ring structure more rigid on one hand, and weakens the ([Py–]N involved hydrogen bond on the other hand. As a result, no significant shift was observed for ν_{12}, and ν_1 only experiences a moderate blue shift. The magnitude of the shift in ν_1 is in an order of $CHI_3 > CHBr_3 > CHCl_3 > CHF_3$ according to calculation (Tables 1 and 2). The FTIR experiments with pyridine and $CHCl_3/CHBr_3$ in solution of cyclohexane showed a consistent sequence (Figures 1 and 2). A strong correlation was observed between the values of ν_1 and various interatomic distances among [Py–]N, [Py–]H, $[CHX_2–]$X and $[CX_3–]$H, as well as the two bond critical points (BCP1 and BCP2) and the ring critical point (RCP). The percentage of the contribution from the internal coordinate r([Py–]N…H[–CX_3] was also estimated and closely related to the magnitude of ν_1. Moreover, the molecular orbitals of hydrogen bonding complex from HOMO-4 to HOMO were analyzed to explain their roles in the ring vibrations of pyridine. The triangle vibration turns to be much less sensitive to the pyridine involved hydrogen bonding. The sequence in the magnitude of ring breathing vibration frequency blue shift for haloforms is against the sequence of the electronegativity of halogen atoms because the hydrogen bond formation involves the redistribution of both σ and π electrons, as well as the halogen atoms in haloforms acting as electron lone pair donors in [Py–]H…X[–CHX_2] hydrogen bond.

STUDYING OF CETANE-INCREASING ADDITIVES EFFECT ON THE QUALITY OF DIESEL FUEL

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Diesel fuel is one of the most demanded fuel for automobiles [1]. Each customer, depending on the region, chooses the most different additives to fuels, and they, in turn, are regulated both by the accuracy of the dosage and by quantity entering into fuel. In this regard, the plants are made directly to the needs and needs of the customer, in order to qualitatively realize the compounding of fuel.

In the production of diesel fuels, it is necessary to add certain additives to improve its characteristics and achieve the required quality. There are the following types of additives: depressant, cetane-boosting, anti-wear, depressant-dispersant, lubricating, antistatic, antioxidant.

Cetane-boosting additives are designed to improve the inflammability of diesel fuels in the combustion chamber. In domestic practice, they are used very rarely, since the proportion of straight-run diesel fractions with a high cetane number (TCH) is high in the fuel balance of the country. Highly aromatic middle distillate fractions of various origins

Table 1. Process conditions

Temperature, K	Pressure, atm	Distance between molecules, Å
298	1	4

Table 2. Energy of interaction of the additive with isoparaffins

Component of diesel fuel	E, kkal/mole	E, kJ/mole • K'
Isopropylnitrate	73.74	308.54
3-ethyldecane	238.83	999.29
isopropylnitrate + 3-ethyldecane	328.20	1373.20
Δ	15.61	65.34
2,2,4,4,6-pentamethylheptane	237.40	993.30
isopropylnitrate + 2,2,4,4,6-pentamethylheptane	327.24	1369.18
Δ	16.09	67.32
2,5-dimethylundecane	257.28	1076.45
isopropylnitrate + dimethylundecane	347.09	1452.22
Δ	16.06	67.22
5-buthylnonnan	257.67	1078.12
isopropylnitrate + 5- buthylnonnan	347.32	1453.20
Δ	15.90	66.52
4,5-diethyloctane	238.11	996.27
isopropylnitrate + 4,5- diethyloctane	328.06	1372.60
Δ	16.20	67.78